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COMPUTER SIMULATION STUDY OF THE ENTROPY OF A ½<111>{110} EDGE DISLOCATION IN B.C.C. IRON

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The aim of the theoretical investigation presented here is to extend our knowledge concerning the entropy of a ½<111>{110} edge dislocation in b.c.c. iron. Overcoming the Peierls-Nabarro stress is one of the dislocation mechanisms which have been proposed as rate-controlling during the deformation of b.c.c. iron at low temperatures. Although the changes in entropy associated with this process are usually assumed to be very small, this assumption may be questionable for dislocation processes which are directly related to the properties of the dislocation core.

The calculation of the dislocation core structure is based on the method suggested by Sinclair (1)(2). The computational block is divided into two regions. Region I contains the core where the interactions between the atoms have to be considered explicitly since the continuum theory does not apply. In the remaining region II of the crystallite, continuum theory is assumed. Approximately 4000 atoms are arranged in a b.c.c. crystallographic configuration and embedded in an elastic continuum. The dislocation is of the edge type with Burgers vector ½<111> lying on a {110} plane. It is introduced in the block by submitting each atom in it to the displacements predicted by anisotropic elasticity theory taking into account the higher order terms in the displacement formulae derived by Eshelby (3).

A fast method developed by Sinclair and Pollard (4) of finding equilibrium configurations has been applied assuming that if the displacements from equilibrium are small, the forces are linear function of the displacements. The pair-wise interatomic forces are derived from an interatomic potential developed by Johnson (5).

The Peierls stress τ_p has been calculated using the method originally suggested by Nabarro (6). In order to compare the core structure calculated in a computer simulation study with the Peierls-Nabarro model, Vítek (7) interpreted the core structure as a continuous distribution of the Burgers vector on the plane onto which the inelastic displacements are mostly confined. A homogeneous shear strain corresponding to this stress was imposed upon the configuration and larger stresses were built up by application of small increments until a critical shear stress was reached. The application of an external shear stress acting on the (110) plane in the direction $[\bar{1}11]$ was simulated in the same way as by Basinski et al. (8) and Duesbery et al. (9).

The normalized velocity autocorrelation function (10) can be written as:

$$\Theta(t)= \frac{M}{3NkT} \Sigma_i^N \frac{1}{\Delta t} \int dt' \, \vec{v}_i(t') \cdot \vec{v}_i(t+t'), \tag{1}$$

where $\vec{v}_i(t)$ is the velocity of the i-th particle at time t and where Δt represents the time step in a computer simulation calculation in which the particle velocities at any time are readily available.

One can relate the correlation function to the so-called spectra of the process according to:

$$g(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \Theta(t) e^{i\omega t} dt. \tag{2}$$

Substitution of eq.(1) into eq.(2) yields:

$$g(\omega) = \frac{M}{3NkT} \Sigma_i^N \frac{2\pi}{\Delta t} |\vec{v}_i(\omega)|^2, \tag{3}$$

where

$$\vec{v}_i(\omega)= \int_0^\infty e^{i\omega t} \vec{v}_i(t) dt. \tag{4}$$

To evaluate the harmonic free energy F in the Debye approximation the sum over the normal modes ω_K is transformed to integrals over ω:

$$F = \Sigma_K f(\omega_K) = \int_0^{\omega_L} f(\omega)\ g(\omega)d\omega, \tag{5}$$

where the number of allowed states with frequencies between ω and $\omega+d\omega$ is $g(\omega)d\omega$.

For an ensemble of quantum harmonic oscillators with the frequency distribution function normalized by

$$\int_0^{\omega_L} g(\omega)d\omega = 1 \tag{6}$$

and with $3N_{AV}$ degrees of freedom per mole, we find for the entropy:

$$S = 3N_{AV}\ k\int_0^{\omega_L} d\omega g(\omega)[\frac{\hbar\omega}{kT}\ (e^{\frac{\hbar\omega}{kT}} - 1)^{-1} - \ln(1 - e^{-\frac{\hbar\omega}{kT}})]. \tag{7}$$

In the expression of the entropy we are neglecting the conduction-electron free energy in the case of metals, the effects of anharmonicity and the temperature dependence of $g(\omega)$.

The computation to obtain the vibrational entropy was affectuated over an interval of 800 time steps. The first 200 steps at 10^{-14} sec per step were done as equilibration period of the dislocated lattice. The last 600 steps at 10^{-15}sec per step were used to obtain $g(\omega)$.(eq.1,2). Since the lattice could relax during time steps the evaluation of the vibrational entropy term of the dislocated lattice at the top of the Peierls barrier is a more complicated problem compared to the situation of the dislocation lying in the valley. To tackle this situation homogeneous shear strain corresponding to τ_P was imposed upon the configuration and the velocity vector of each atom in the crystallite was calculated over 800 steps at 10^{-16} sec per step.

The frequency spectra of the stressed and unstressed slipsystem are shown in Fig. 1. Once the frequency distribution curve is known the vibrational entropy can be calculated using eq.7. Fig. 2 shows the curve $T\Delta S$ where ΔS means the difference between the entropy of the stressed and unstressed dislocated lattice.

The predominant internal change due to an applied shear stress is the widening of the core which occurs by a movement of the edge dislocation. Some redistributions take place within the fractional dislocations lying near the centre of the edge dislocation but these do not seem to be very important. The Peierls stress is 0.004μ where μ is the shear modulus for shear in the [T11] direction. The Peierls stress obtained (11) using the method of Vítek et al. (7) is somewhat lower (12) than calculated using the procedure originally suggested by Nabarro (0.005μ)(6).

The results of the Peierls stress appear to yield reasonable values, which are in agreement with the results of the investigations of Kossowsky (13)(14). The calculations carried out by Vítek and Yamaguchi (15) are in conformity with the present results.

Assuming that flow and yielding are each controlled by a thermally activated deformation process one has to take into account the activation entropy. For thermally activated mechanisms involving elastic distortions two contributions to the entropy factor can be expected on purely theoretical grounds. ΔS_{vibr} arises from the changes in the frequency distribution curve as the activated configuration reaches the saddle point. The second contribution $\Delta S_{elastic}$ originates from the temperature dependence of the elastic modulus.

Schoeck (16) made an analysis of the thermodynamic quantities and he found (17)(18) $T\Delta S_\mu = (\mu_0-\mu_T)\Delta H_0/\mu_0$, where μ_0 and μ_T are the shear modulus at 0°K and a given temperature T, respectively and $\Delta H_0(\simeq 0.08\ b^3)$ is the activation enthalpy at zero effective stress. Using Schoeck's expression and the values of the elastic constants given by Rayne et al.(19). ΔS_μ is 3.7 J/mole °K at T = 90°K. The Schoeck's entropy term ΔS_μ is only an approximation to the entropy which can be determined from the normalized vibrational spectrum of the unstressed slipsystem (Fig. 1). The entropy term for the unstressed case is equal to 4.9 J/mole °K at T = 90°K.

The curve $T\Delta S_{vibr}$ vs. T (Fig.2) exhibits a minimum value of -22.7 J/mole at T = 92°K. The frequencies can be expected to increase as a result of the higher stiffness associated with the saddle point positions. ΔS_{vibr} has a negative value.

Altshuler and Christian (20) investigated the mechanical properties of pure iron tested in compression over the temperature range 2 to 293°K. The rate theory analysis showed a variation with the temperature of ΔH. On purely theoretical grounds we may conclude that the contribution of the entropy to the total free energy is at most 5% of the activation enthalpy in the low temperature region. The results presented here appear to be in reasonable agreement with the experimental data which demonstrate that there is at present no convincing evidence for any considerable activation entropy.

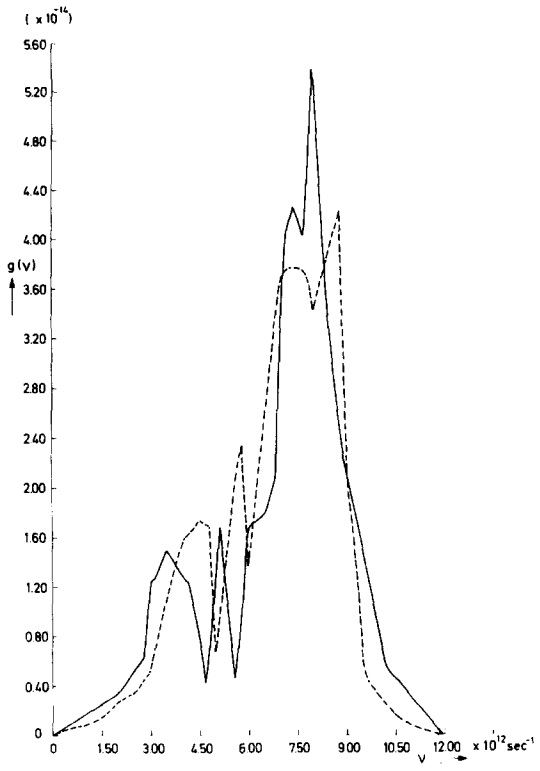

FIG. 1

The normalized vibrational spectra of the stressed (broken line) and unstressed slip system $\frac{1}{2}\langle 111\rangle\{110\}$.

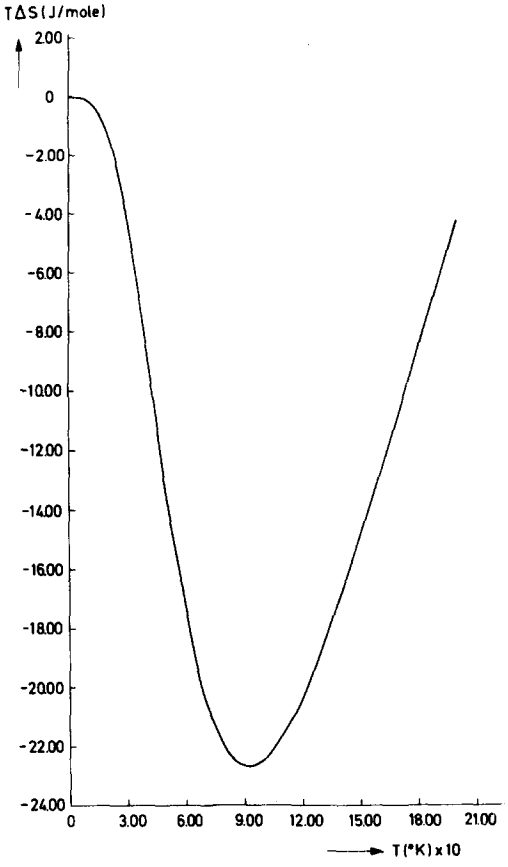

FIG. 2

TΔS vs. T curve where ΔS is the difference between the vibrational entropy of the stressed and unstressed lattice.

The method described to compute the vibrational entropy of a solid appears to be an appropriate procedure for imperfect crystals. The accuracy depends on one's knowledge of the interatomic potential. With Johnson's potential, the Debye temperature Θ_D ($\nu_{max} \simeq 9\ 10^{12}$ Hz for the $[\zeta\zeta\zeta]$ branch of the phonon dispersion curve) is 432°K. This is in fair agreement with the value of 460°K given by Brockhouse et al. (21). However, it may be noted that the truncation process inevitable in having to choose finite intervals for the transformations involved (eq.(4), eq.(6)) could introduce artifacts. Especially, the tail of higher frequencies (Fig.1), greater than 10^{13}sec^{-1}) is generated by making use of eq.(6) over a finite period of time. Work is in progress to apply non-equilibrium statistical mechanics developed by Progogine (22) to obtain the vibrational entropy of a dislocated lattice lying at the top of the Peierls barrier.

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